ALCF Early Science Program

Argonne NATIONAL LABORATORY

ESP Kick-Off Workshop
Project Plan Presentation

Lattice Quantum Chromodynamics

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for USQCD

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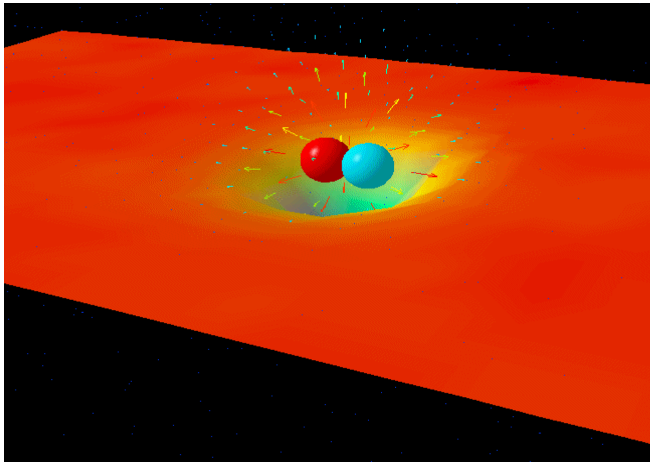


Lattice QCD

Scientific Field:
Nuclear & High Energy Physics

QCD is the fundamental theory of strong nuclear interactions, the theory of quarks and gluons.

Lattice QCD is a method for solving the theory with numerical simulations by formulating it on a four-dimensional space-time lattice.

Invented by Ken Wilson in 1973. Wilson was also instrumental in pushing the field of scientific supercomputing, and establishing the network of NSF centers for scientific supercomputing; LQCD has made heavy use of scientific supercomputers from the start.

GOALS:

Determine basic parameters of the standard model of particle physics.

Compute masses, decay properties and internal structure of strongly interacting particles.

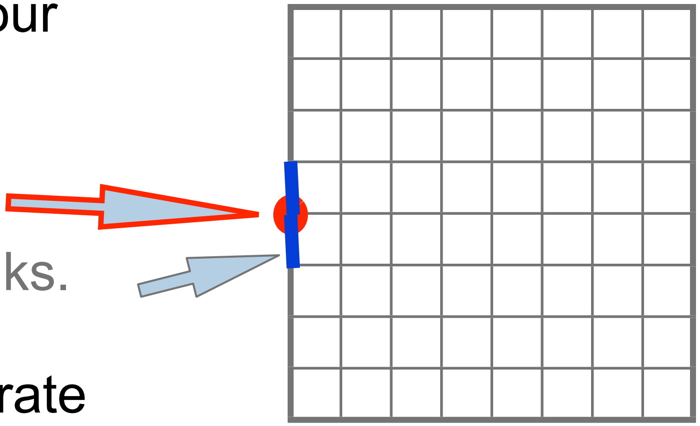
Obtain a quantitative understanding of the behavior of strongly interacting matter under extreme conditions of temperature and density.

Begin the study of strongly interacting theories that may be necessary to explain electroweak symmetry breaking under investigation at the LHC.

Lattice quantum field theories

Approximate the path integral of quantum field theory by defining the fields on a four dimensional space-time lattice.

Quarks (ψ) are defined on the sites of the lattice, and gluons (U_μ) on the links.



Monte Carlo methods are used to generate a representative ensemble of gauge fields.

- **E.G., Hybrid Monte Carlo algorithm:**
  - Multi-time step Hamiltonian evolution

The Dirac operator

The fundamental operation that consumes the bulk of our cycles is the solution of the Dirac equation on the lattice (a large, sparse, linear system).

Quarks in QCD come in three colors and four spins.
The color covariant Dirac operator of lattice QCD is

$$D_\mu \gamma_\mu \psi(x) \equiv \frac{1}{2}\left(U_\mu(x)\gamma_\mu\psi(x+\hat{\mu}) - U_\mu^\dagger(x-\hat{\mu})\gamma_\mu\psi(x-\hat{\mu})\right)$$

γ operates on spin four-vector.

U operates on color three-vector of the quark.

Relaxation methods are used to calculate the propagation of quarks through the gauge field.

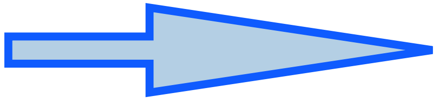
Repeated solution of Dirac equation

– at each step of the HMC algorithm

Anatomy of a typical lattice calculation

Generate gauge configurations on a leadership facility or supercomputer center.
Tens of millions of BG/P core-hours for single ensemble.

A single highly optimized program, very long single tasks.
Needs high capability computing.



Transfer to labs for analysis on clusters.
Comparable CPU requirements.

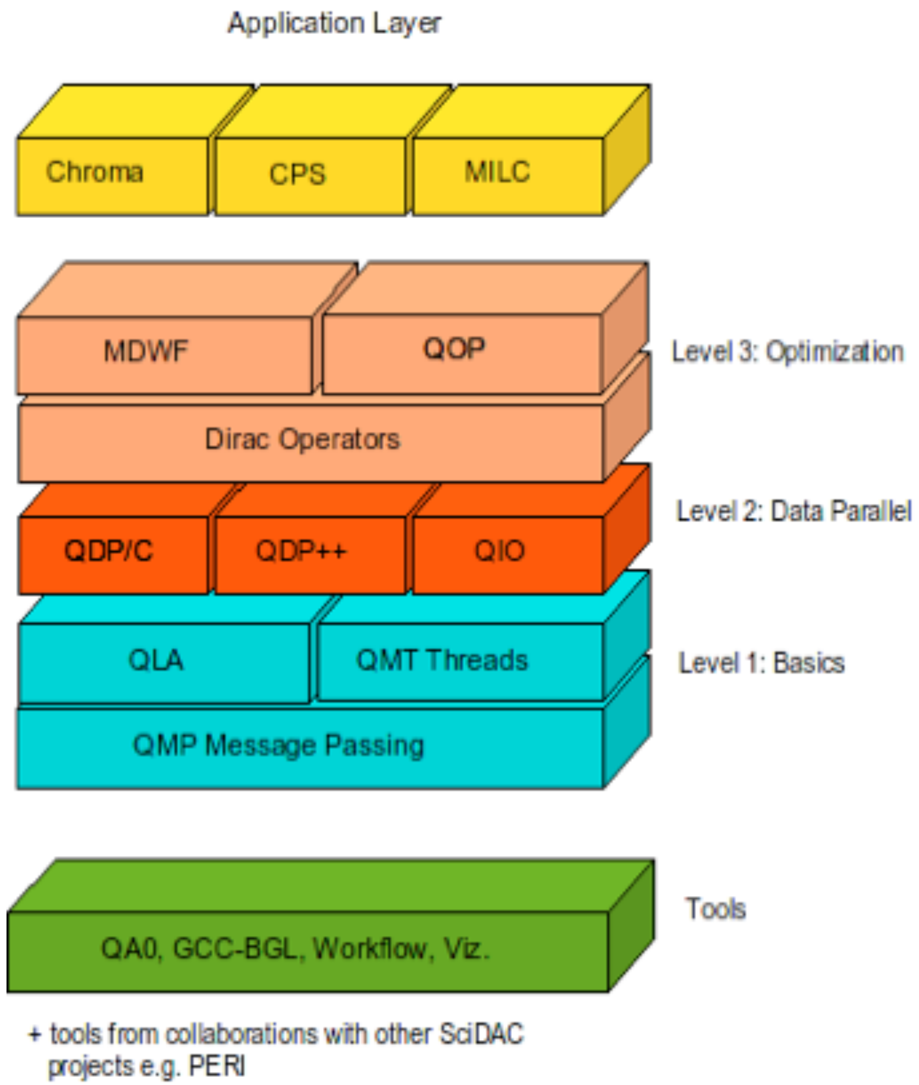
Large, heterogeneous analysis code base, 10,000s of small, highly parallel tasks.
Needs high capacity computing.

- **First computational goal on BG/Q: generate state-of-the art gauge configuration ensembles, release to community.**
  - Mira enables using physical values of light quark (up, down) masses. Currently can only use heavier quark masses (Intrepid).
  - Mira enables finer lattice spacing than current runs on Intrepid. Finer lattice spacings help extrapolate to continuum limit to obtain physical results.

Library and tools

Codes: MILC, Chroma, CPS

- QCD SciDAC API for Chroma/ CPS/MILC applications
- Level 3: Highly Optimized Dirac inverter, other critical kernels
- Level 2: Data Parallel Interface & IO library
- Level 1: Single core linear algebra, message passing, and threading libraries.
- Specialized code generators, workflow, etc.



Participants in USQCD software development

Arizona	Doug Toussaint	MIT	John Negele
	Alexei Bazavov		Andrew Pochinsky
BU	Rich Brower *	North Carolina	Rob Fowler*
	Ron Babich/Mike Clark		Pat Drayer
	James Osborn (ANL)	JLab	Chip Watson *
BNL	Chulwoo Jung		Robert Edwards *
	Oliver Witzel		Jie Chen
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Columbia	Bob Mawhinney *	IIT	Xien-He Sun
DePaul	Massimo DiPierro	Indiana	Steve Gottlieb
FNAL	Don Holmgren *		Aaron Turok
	Jim Simone	Utah	Carleton DeTar *
	Jim Kowalkowski		Tommy Burch
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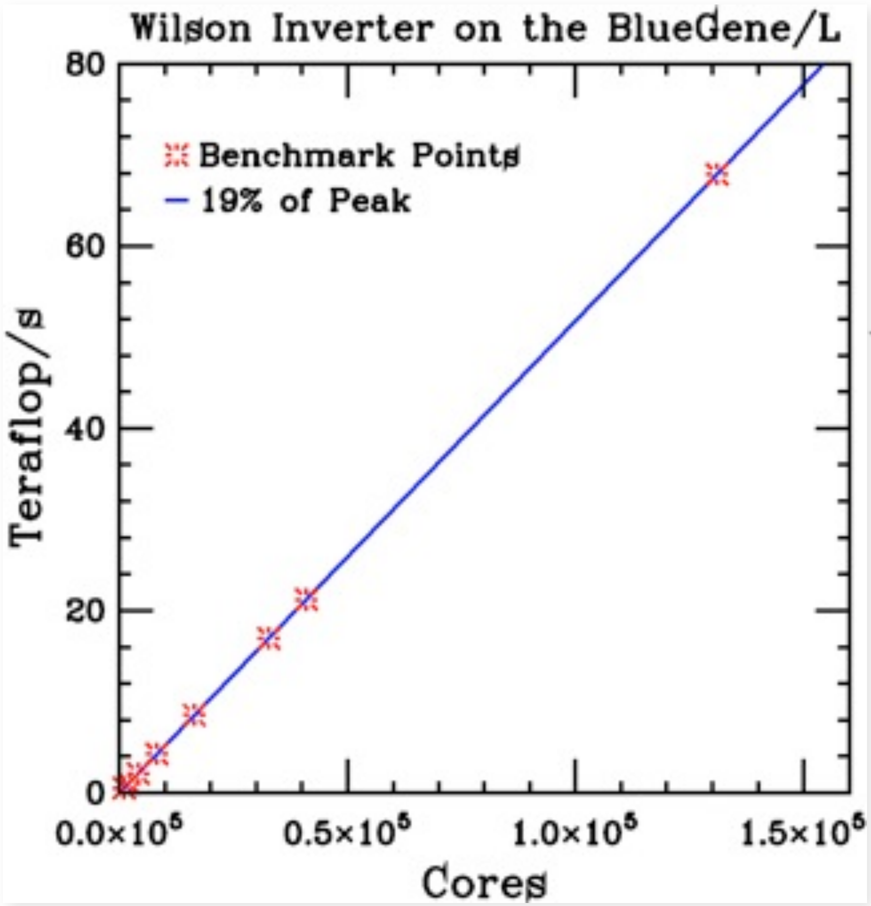
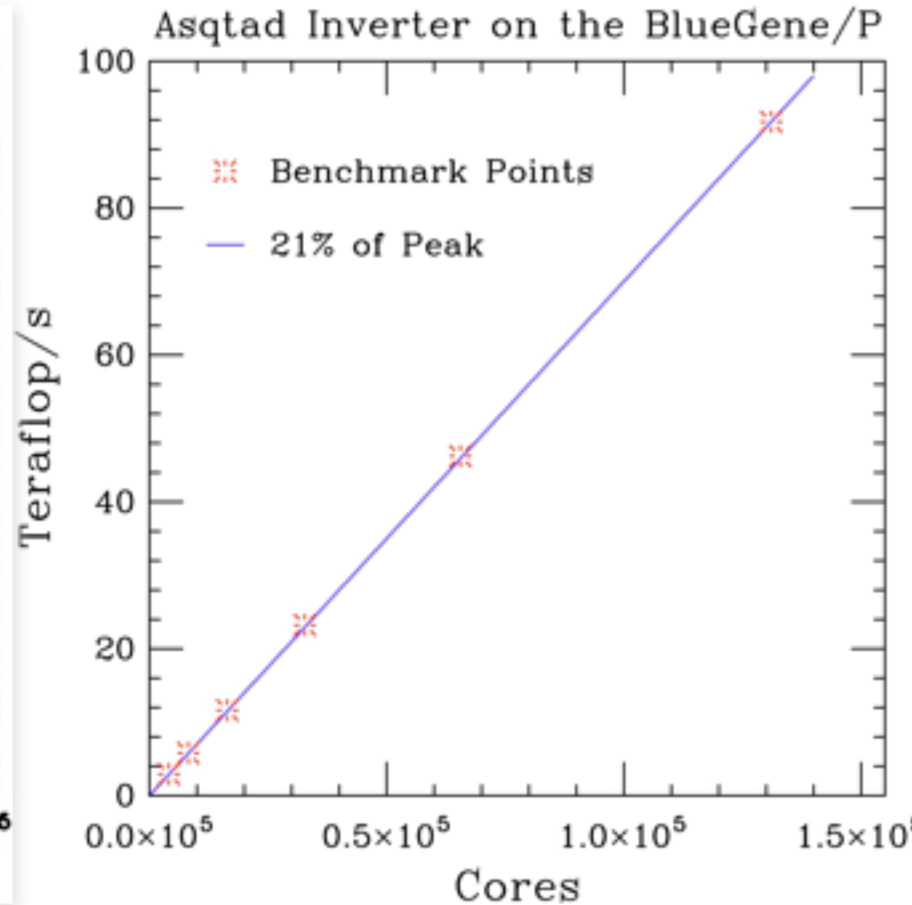
LLNL	Pavlos Vranas*		Ted Bapty

* Software Committee: Participants funded in part by SciDAC-1 & 2

Parallelism and weak scaling





Weak scaling for Wilson Fermions on the BG/L (2006 Gordon Bell award) and for Asqtad on the BG/P, both up to 131,072 cores.

USQCD/IBM co-design efforts

- **As part of USQCD and UKQCD projects, a team from Brookhaven, Columbia University and the University of Edinburgh has been working as IBM contractors on BG/Q for the past four years.**
  - Designed the prefetching interface between the processor and L2 cache in the BG/Q. (Boyle/Christ/Kim)
  - Important feedback from QCD code performance to memory system design.
  - LQCD code was the first high-performance application code to run on the fullchip simulator.
  - Dirac matrix inversion kernel presently gets 60% of theoretical peak on BG/Q chip. (Peter Boyle)
  - Dirac matrix inversion kernel now running over MPI on 128 BG/Q nodes
  - Full hybrid Monte Carlo evolution code now running on a single BG/Q chip. (Chulwoo Jung)

Plan for next 6 months

- Optimize communication for high performance Dirac inversion code (Boyle).
  - QCD now running on 512-node BG/Q hardware (with non-optimized communications).
  - Code fragments exceed 80% of peak communication bandwidth.
- Optimize threading of code generating gauge configurations (Jung).
  - OpenMP code now running single node.
  - Add communications and optimize threading.
- Complete high performance parallel transport and create high performance staggered inverter (Boyle/Jung).
- Begin production running on 512 node prototype hardware at Yorktown.
- Port QLA, QMP, QDP, and QMT to BG/Q
  - Prototype ports of QMP and QDP have been used in code mentioned above.
- Continue development and begin porting of improved algorithms (force-gradient integrator, domain decomposition, multi-grid).